A NETWORK MODEL FOR TRANSPORT OF BACTERIA THROUGH SATURATED POROUS MEDIA

By

Neeru Jaiswal

ENVIRONMENTAL ENGINEERING AND MANAGEMENT PROGRAMME
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CERTIFICATE

This is to certify that the thesis entitled "*A Network Model for Transport of Bacteria Through Saturated Porous Media*" by Neeru Jaiswal is a record of the work carried out by her under my supervision and that the work has not been submitted elsewhere for a degree.

Date: 16.07.2003

(Saumyen Guha)

Assistant Professor
Department of Civil Engineering
Indian Institute of Technology Kanpur

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Abstract

A two-dimensional network model for porous media was developed to simulate the transport of bacteria through saturated porous media. The model was a regular square network consisting of pore throats or tubes with randomly distributed radii from Weibull distribution. The length of the pore throat was calculated by equating the porosity of the porous media with that of the network. The network thus obtained simulated the reported results of drainage capillary pressure curve for porous media. Given the heads at the inlet and outlet, head at each node was computed by repeated applications of Darcy-Weisbach equation in the network and solving the system of non-linear equations using the Newton-Raphson method. The hydraulic model was validated by hand-computed values in simple networks. The particle transport model was incorporated by repeated application of Iwasaki equation to each tube in the network with the assumption that the filter coefficient is constant in a small tube during a small time step. Using the mass balance equation, deposition in the tubes was also computed. The filter coefficients and velocities in the tubes were updated at each time step using the deposition values. The transport model was checked for consistency by simulating for conservative tracer. The simulation results for a non-conservative particle (bacteria) transport shows similar qualitative trends as reported for bacterial transport column experiments. The effects of various distribution parameters and grain sizes on the pore throat (tube) radii distribution are discussed. The model was then used to study the effects of various parameters such as, porosity, flow rate, adhesion efficiency (α), maximum specific deposit (σ_{max}) etc. on breakthrough curves. The adhesion efficiency (α) was found to be a critical parameter that can significantly alter the transport.

List of Symbols

$A_{bs(w)}$ = Hamaker constant for Van der Waals interaction between a bacterium (b) and solid phase (s) across the medium water (w).

B = blocking factor

C = particle mass concentration in the fluid phase

C_0 = initial influent particle concentration

C_{0t} = influent particle concentration at time t

D_b = diffusion coefficient of the bacterium

F_t = cumulative density function for pore throat

F_b = cumulative density function for pore body

H_k = head at the kth node,

K_{ki} = head loss coefficient for the pipe connecting the nodes k and i

N_G = gravity settling parameter

N_{Pe} = peclet number

N_R = relative size parameter

N_t = total number of tubes in the network.

N_{vdw} = Van der Waals attraction parameter

Q_{ki} = flow in the pipes connecting the nodes k and i

R_i = radius of ith tube

R_{ki} = radius of the tube connecting nodes k and i

U_i = consumptive use at node I

a_b = radius of bacterium

a_s = radius of the media particle

$b_{t\,min}$ = minimum pore throat sizes

$b_{t\,max}$ = maximum pore throat sizes

$b_{b\,min}$ = minimum pore body sizes

$b_{b\,max}$ = maximum pore body sizes

f = friction factor

g = gravitational acceleration

h_{ki} = head loss in the tube connecting nodes k and i

h_n = number of horizontal nodes,

l = length of one tube

m_i = number of connections to node i

n_{ki} = exponent in the head loss equation for the pipe connecting nodes k and i.

s = scouring coefficient.

v = updated velocity in the tubes

v_0 = initial velocity in the tubes

v_{ki} = velocity in the tubes connecting the nodes k and i

v_n = number of vertical nodes

x = distance along the direction of flow

x' = positive empirical parameters

y' = positive empirical parameters

z' = positive empirical parameters

α = adhesion or clean bed collision efficiency

α_0 = clean bed collision efficiency

α_b = parameters of the Weibull distributions for the pore body

α_t		= parameters of the Weibull distributions for the pore throat
β_b		= parameters of the Weibull distributions for the pore body
β_t		= parameters of the Weibull distributions for the pore throat
β		= positive empirical parameters
ε		= porosity of the network at time t,
ε_0		= initial porosity of media
η		= mass transfer efficiency
λ_0		= Clean bed filter coefficient
λ		= filter bed filter coefficient at time t and space x
μ		= dynamic viscosity of the fluid phase and
θ		= fraction of surface covered, i.e. the number of the cells
θ_{max}		= maximum surface coverage
ρ_f		= fluid density
ρ_p		= particle (bacteria) density
σv		= volume of deposit per bed volume
σ		= mass of deposit per bed volume
$\sigma_{v\ mav}$		= volume of maximum deposit per bed volume

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Chapter 1

Introduction

Frequently ground water is used without treatment because of the perceived filtering action of solution flow through porous media. It is now recognized, however, that bacteria and viruses can travel considerable distances in aquifers and saturated soils, thus posing a contamination threat to surface waters and well waters (Bouwer, 1984). Historically, bacterial contamination of ground water can be associated with the age-old practices of traditional septic tank disposal systems and land application of sewage sludge (Gerba and Bitton, 1984). However the concern over microbial quality of ground water supplies is fairly recent. A number of field studies have indicated that many waterborne epidemics owe their origin to bacterial contamination of ground water (Wilson et al., 1983, Romero, 1970). It is well established that, microbial contamination occurs when human wastes enter the soil, since microbes can travel long distances through aquifers under appropriate conditions (Corapcioglu and Haridas, 1984). A large number of outbreaks of water-borne disease have been attributed to contaminated groundwater (Gerba and Bitton, 1984). Control of microbial transport and retention in porous media is also required for effective and safe bioremediation (Bouwer, 1993). Thus the study of bacterial transport is of paramount importance, in order to determine whether the bacteria, introduced to the subsurface reach the point of interest.

Bacterial mobility through a porous medium depends on a number of processes such as, advection, dispersion, attachment, detachment, etc (Smith et al., 1985; Harvey et al., 1993). Body forces arising due to gravity, buoyancy, hydrodynamic drag, Van-der-Waals interaction, double layer interaction and hydrophobic interaction affect the

transport, attachment and detachment of bacteria (Rajagopalan and Tien, 1976). Natural heterogeneity of porous media adds further complexity to the transport process (Fontes et al., 1991; Harvey and Garabedian 1991). As a result, mechanistic models for complete bacterial transport that takes into account the effects of individual processes and forces are non-existent. Large-scale transport models often consider bacterial retention on the porous media either as an equilibrium process or as a first order kinetic process, devoid of any mechanistic description of individual forces (Corapcioglu and Haridas, 1984). Attempts to incorporate the mechanisms of bacterial retention on porous media typically consider the process to be a combination of transfer of bacteria from bulk water to the collector surface (mass transfer efficiency) and adhesion (collision efficiency). The mass transfer efficiency was simulated (Rajagopalan and Tien, 1976; Basu, 2001) using the sphere-in-cell porous media model (Happel, 1958). This lead to initial collection efficiency when the collision efficiency was assumed to be unity. Validation of these models requires computation of initial collection efficiencies from the breakthrough curves obtained from laboratory column experiments for comparison with the model simulations. Computation of the initial collection efficiency from discrete time series (experimental breakthrough curve) can be cumbersome and introduce transformation errors (Rijnaarts et al. 1996).

A model that incorporates the physical processes as well as capable of directly simulating the breakthrough curve will be helpful in predicting laboratory column experiments results under changing physical parameters. Such a model will be a robust tool for design of experiments and prediction of qualitative effect of different physical parameters on bacterial transport. Goal of the present work is to develop a 2-D network model for bacterial transport through porous media under saturated flow condition that

qualitatively simulates the changes in breakthrough curves obtained from laboratory column experiments under changing physical parameters.

The thesis has been organized as follows:

Chapter 2 gives the status of the literature on the related areas.

Chapter 3 states the scope of the work.

Chapter 4 outlines the development of the model.

Chapter 5 describes the results obtained from the simulations and compares with the reported experimental results.

Chapter 6 summarizes the work and states the key conclusions.

Chapter 7 lists the scope for future work.

Chapter 2

Literature Review

2.1 Modeling of Micro-structure and Fluid Flow through Porous Media

The earliest studies of fluid flow through porous media used the sphere pack as model. Kozney (1927) and Carman (1938) derived an equation, which related permeability of porous media to porosity and internal surface area of sphere pack. Rapport and Leas (1952) reduced the porous medium to an equivalent bundle of tubes through many assumptions. Many frequency distributions were proposed that related the properties of porous media to the radii of the equivalent bundle of tubes (Childs and Collis-George, 1948; Gates and Tempelaar Leitz, 1950; Fatt and Dykstra, 1951; Purcell, 1949; Burdine, et al., 1950). Several obvious characteristics of real porous media are not present in the bundle of tubes model. The major weakness of the bundle of tubes model lies in the absence of cross-connections between the tubes. An examination of thin sections of sandstone indicated that the cross connections between pores was a major structural feature of the porous media (Fatt, 1956). The sphere pack model did have interconnected pores, but the shapes of these pores were so complex that no analysis of flow through them was possible. If the two models are combined by substituting a uniform cylindrical tube for each pore space in the sphere pack model, a three dimensional network of tubes is obtained on which, in principle, exact flow calculations can be made (Fatt, 1956).

2.2 Network Model

Network models represent an interconnected network of capillary tubes within a porous media. The lattice of cubic chambers and rectangular tubes of the network represent the pore bodies and the pore throats respectively. These models can be used to

construct a picture of the microscopic phenomena in a porous medium and serve as a tool for analyzing experimental and theoretical concepts.

The use of network model is not new in the world of modeling of flow through porous media. Such models are used in petroleum engineering, chemical engineering and physics and increasingly in hydrology (Reeves and Celia, 1996). These models are now heavily used as investigative tools to study the nature of fluid flow from the perspective of the pore scale. Majority of the studies have been limited to multi-phase fluid flow in porous media. In groundwater hydrology, many such applications were reported for pressure-saturation relationship for unsaturated fluid flow (Reeves and Celia, 1996; Held and Celia, 2001). However, no study so far has been reported for the particle transport through porous media under saturated condition using the network models.

Network models of pore structure were first pioneered by Fatt (1956) based on the idea that pore space may be represented as an interconnected network of capillary tubes whose radii represent the dimension of pores within a porous medium. One of the early attempts was the work of Chatzis and Dullien (1977), who applied bond percolation to regular two-dimensional and three-dimensional lattices. Several attempts to develop porous media models have been reviewed (Payatakes and Dias, 1984; Dullien and Batra, 1970).

To simplify the network operations, it is desirable to replace the three-dimensional network by a two-dimensional network. In terms of the porous medium the replacement is justified by assuming that a very thin slice of porous medium with impermeable planes sealing the two large surfaces has the same properties as a cube of the same material. This is equivalent to assuming that the change produced by making

the porous medium thin, and thereby eliminating a number of cross-connections in the third dimension, may be compensated by introducing additional channels within the two-dimensional network. It is also assumed that changes in the tube radii distribution, network configuration and other variables influence the properties in the same qualitative manner in the two dimensional network as in the three dimensional network (Fatt, 1956). For single-phase flow, "blind" or "dead end" pores in the porous medium are assumed to be absent. There is very little experimental information on the existence of blind pores in real porous media.

2.2.1 Spatial Distribution of Tubes

The network model generally chosen to represent the porous media is a regular network lattice having nodes in X and Y directions respectively. The nodes of lattice represent the pore bodies; each node is connected with pore throats, which are represented by bond of the lattice. The only parameter used to describe the network configuration is the number of tubes connected to each tube. This parameter is typically called the β-factor. Many different regular networks can be chosen (Fatt, 1956). Some of these are shown in Figure 2.1 and their β-factors are tabulated in Table 2.1.

Table 2.1 β-factors for four networks shown in Figure 2.1.

Network	β Factor
Single hexagonal network	4
Square network	6
Double hexagonal network	7
Triple hexagonal network	10

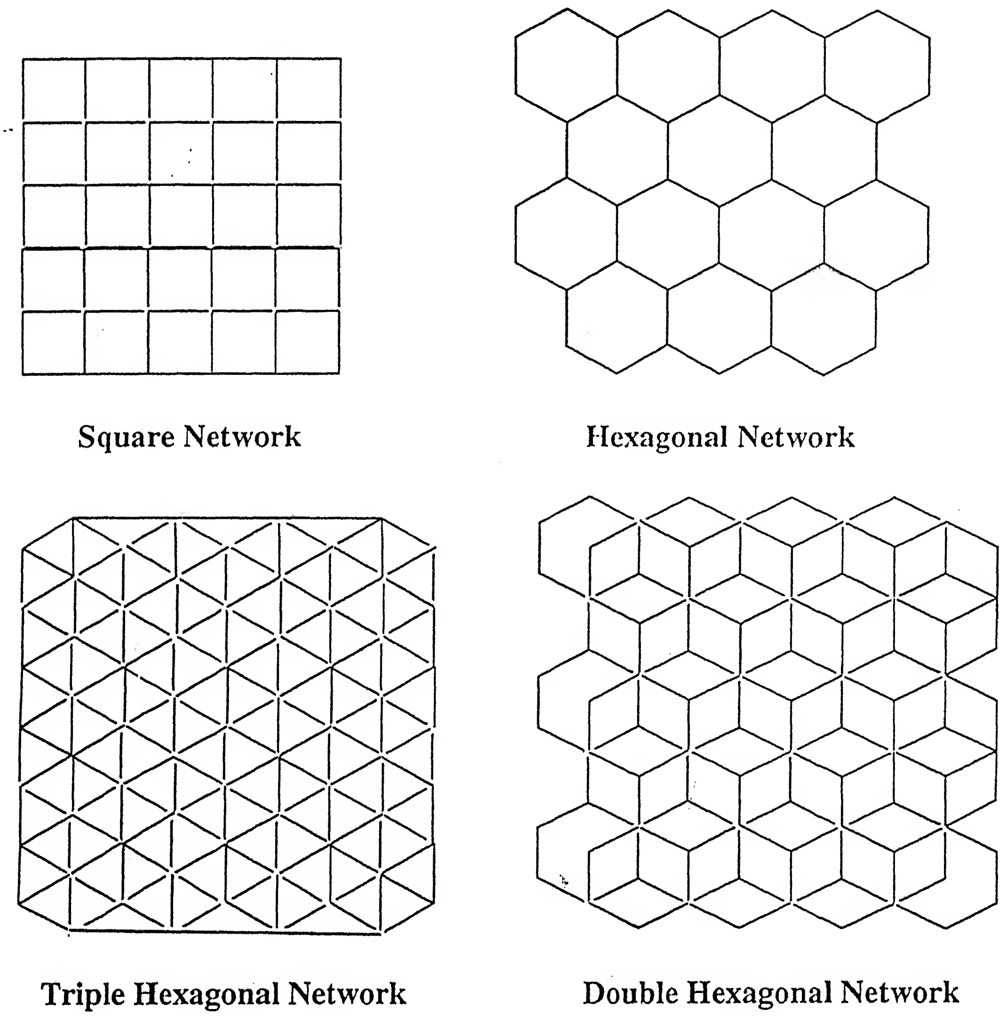

Figure 2.1 Different types of network used for the description of pore network in a porous media (Fatt, 1956).

2.2.2 Pore Size Distribution

To this end the most realistic models for porous media are those which approximate the pore space as a network of pores in which relatively larger pores (pore bodies) are connected by relatively narrow pores (pore throats). Existing pore size determination techniques (eg. Mercury porosimetry) provide information only about an equivalent capillary size, which is heavily weighted towards the smallest pore throat dimension (Jenkins and Rao, 1984; Dullian and Dhawan, 1974). Ioannidis and Chatzis (1993) presented a methodology for estimating pore throat and pore body size distribution of a large class of porous media for use in the network model. For the network model to be

geometrically defined, dimensions of all pore bodies and pore throats must be determined. It is assumed that the pore throat and pore body characteristic dimensions, b_t and b_b follow Weibull distributions, f_t and f_b respectively. These are generally defined as follows (Ioannis and Chatzis, 1993):

$$f_i(b_i) = \left(\frac{\beta_i}{\alpha_i}\right)\left(\frac{b_i - b_{i\,\min}}{\alpha_i}\right)^{\beta_i - 1} F_i(b_i), \quad i = b,t \tag{2.1}$$

$$F_i(b_i) = \frac{\exp\left[-\left(\frac{b_i - b_{i\,\min}}{\alpha_i}\right)^{\beta_i}\right] - \exp\left[-\left(\frac{b_{i\,\max} - b_{i\,\min}}{\alpha_i}\right)^{\beta_i}\right]}{1 - \exp\left[-\left(\frac{b_{i\,\max} - b_{i\,\min}}{\alpha_i}\right)^{\beta_i}\right]} \tag{2.2}$$

where,

$b_{t\,\min}$ = minimum pore throat radius,

$b_{t\,\max}$ = maximum pore throat radius,

b_t = random number obtained from the distribution,

α_i and β_i = parameters of distribution.

Once the frequency distributions f_t and f_b are selected, pore sizes b_t and b_b are assigned to the nodes and bonds of the network according to the bond-correlated site percolation scheme (Diaz et al., 1987). The pore throat, are not distributed randomly over the network, but are correlated to the pore bodies that are randomly distributed. This correlation is expressed by the following equation (Chatzis, 1980):

$$F_t(b_t) = F_b^2(b_b). \tag{2.3}$$

The physical significance of this correlation is that, large pore throats are associated with the large pore bodies. Such correlations have been experimentally observed by Wardlaw et. al. (1979). In the construction of the network model the node-to-node

distance (l) is adjusted so that the porosity of the network is equal to the porosity of the porous media under consideration.

2.2.3 Simulations Using Network Model

Network models of pore structure, based on bond-correlated site percolation concepts, were successfully used to predict the drainage capillary pressure curves for mercury-air and oil-water displacements, absolute permeabilities and formation resistivity factors of sandstones (Ioannidis and Chatzis, 1993). Reeves and Celia, 1996 used pore scale network model to determine quantitatively a macroscopic relationship between capillary pressure, fluid saturations, and interfacial area between fluid phases. Network model have been used to study diffusion and dispersion (Hollewand and Gladden, 1992; Burganos and Payatakes, 1992; Koplic et al., 1988), pore-scale evaporation process (Nowicki et al., 1992), the formation and flow of foam (Laidlaw et al., 1993), the interpretation of mercury porosimetry and associated characterization of pore size distributions (Ionnidis and Chatzis, 1993; Chatzis and Dullien, 1985), and ganglion formation and mobilizations (Dias and Payatakes, 1986). There have been several network model developed to study the constitutive relationships required to parameterize multiphase flow equations. The relative permeability-saturation function has been studied, primarily by petroleum engineers (Bryant et al., 1993; Blunt and King, 1991; Kantzas and Chatzis, 1988). The moisture retention function for both two and three phase systems has also received attention (Soll and Celia, 1993; Soll, 1991; Ferrand and Celia, 1989).

2.3 Bacteria Transport Models

Porous media refer to a fixed bed of granular material containing the pores through which a solution may flow. When flowing through porous medium, the particles are

brought into contact with the particle retention sites; they are retained there or are carried away by the stream. Particles that collect on the porous media form a deposit that can alter the fluid flow properties and decrease the permeability.

The mechanisms by which particles in the suspension are removed within a porous media are complex and can be described in three steps: (i) Transport of the particles to the collector surface or mass transfer efficiency (η), (ii) attachment of the particle to the collector surface or adhesion efficiency (α), and, (iii) detachment of particles from collector surface due to hydrodynamic forces. Transport and adhesion are physical processes, which depend on the characteristics of suspended solids (size, shape and density), characteristics of collector (surface area, pore size and shape) and characteristics of flow (velocity, viscosity and temperature).

2.3.1 Models Based on Colloid Filtration Theory

The fundamental equation describing the particle retention in a filter bed is the macroscopic mass conservation equation. The basic filtration equation proposed by Iwasaki (1937) for the particle removal from the solution is as follows:

$$\frac{dC}{dx} = -\lambda_0 C \text{ with } C = C_0 \text{ at } x = 0 \text{ (influent)} \quad (2.4)$$

where,

λ_0 = initial filter bed coefficient.

Solution of Equation 2.4 is,

$$C(x) = C_0 \exp(-\lambda_0 x) \quad (2.5)$$

The equation is only valid for a clean bed, i.e. at the initial stages of filtration. Accordingly, λ_0 is termed as clean bed filter performance coefficient. Initial attempts at relating λ_0 to particle, media, and flow properties were widely divergent since

usually only suspension concentration was measured and influent particle size was poorly known (Ives, 1970). A mechanistic understanding of clean bed filtration has followed advances in the modeling literature (Yao et al 1971; Spielman and FitzPatrick 1973; Payatakes et al. 1974; Rajagopalan and Tien 1976; Tien and Payatakes 1979). These models were primarily based on Happel's spehere in cell model that substitutes a single isolated collector for porous media with a liquid shell around it (Happel 1958). Deposition is controlled by two processes: transfer of particles from bulk water to the collector surface and adhesion. Colloid filtration theory was used to quantify these two processes in terms of the collector mass transfer efficiency λ (the probability of particle approaching a collector to reach its surface) and the adhesion or collision efficiency α (the probability of a particle to attach upon reaching the surface). The trajectory of a particle near the collector surface was obtained by considering various surface and body forces such as, inertial force, gravitational force, drag forces, DLVO forces etc. The mass transfer efficiency or the initial collection efficiency (η) was computed based on the assumption that all the particles that reach the collector surface are attached, i.e., $\alpha = 1$. This initial collection efficiency was approximated well by the following semi-empirical equation (Rajagopalan and Tien, 1976):

$$\eta = 4A_s^{1/3}N_{P_e}^{-2/3} + 0.72A_sN_{vdw}^{1/8}N_R^{15/8} + 2.4\times10^{-3}A_sN_G^{1.2}N_R^{-0.4} \quad (2.6)$$

where,

$$A_s = \frac{1-P^5}{1-\frac{3}{2}P+\frac{3}{2}P^5-P^6}$$

$$P = (1-\varepsilon_0)^{1/3}$$

$$N_{pe} = 2Ua_s/D_b$$

$$N_R = a_b/a_s$$

$$N_G = 2a_b^2(\rho_p - \rho)g/(9\mu U)$$

$$N_{vdw} = A_{bs(w)}/(9\pi a_b^2 U)$$

ε_0 = initial porosity of the column,

U = velocity of the fluid phase,

D_b = diffusion coefficient of the bacterium;

ρ_b and ρ = densities of the bacterium and fluid phase respectively,

a_b = radius of bacterium,

a_s = radius of the media particle,

μ = dynamic viscosity of the fluid phase and

$A_{bs(w)}$ = Hamaker constant for Van der Waals interaction between a bacterium (b) and solid phase (s) across the medium water (w).

The first term on the right hand side of Equation 2.6 describes the contribution of convection and diffusion to η while the other terms account for direct interception and deviation from trajectories due to other influences. This model for η was later modified by Basu (2001) to incorporate the effect of hydrophobic forces. The initial filter performance coefficient (λ_0) was related to the initial collection efficiency (α) as follows (Rajagopalan and Tien 1976):

$$\lambda_0 = \frac{3}{4}\frac{(1-\varepsilon_0)}{a_s}\eta\alpha \qquad (2.7)$$

A complete mass balance of particles requires consideration of accumulation of deposited particles as well as particles in suspension. Assuming uniform flow velocity, negligible dispersion, and small local change in suspended solids concentration, the mass balance expression becomes (Herzig et al., 1970),

$$\frac{\partial \sigma}{\partial t} = -U\frac{\partial C}{\partial x} \qquad (2.8)$$

where,

σ= mass deposited per unit volume of bed,

C= concentration of particles in suspension.

By further considering the scouring of the deposited mass as a first order reaction, one obtains (Herzig, et. al. 1970):

$$\frac{\partial \sigma}{\partial t} = -U\frac{\partial C}{\partial x} - s\sigma \tag{2.9}$$

where,

s = scouring coefficient.

As particles accumulate, the clean bed filter coefficient λ_0 no longer applies and λ changes with the amount of deposition (σ). A phenomenological model that relates the filter coefficient during clogging of deposited particle volume is as follows (Ives, 1970),

$$\lambda = \lambda_0\left[1+\beta\frac{\sigma_v}{\varepsilon}\right]^{z'}\left[1-\frac{\sigma_v}{\varepsilon}\right]^{y'}\left[1-\frac{\sigma_v}{\sigma_{v\max}}\right]^{x'} \tag{2.10}$$

where,

λ = filter bed coefficient at time t,

ε = porosity at time t,

$\sigma_{v\,max}$ = maximum deposit volume per bed volume,

σ_v = volume of deposit per bed volume.

β, x', y' and z' are positive empirical parameters evaluated from specific filtration data.

The Equation 2.10 is based on the three processes: an increase in the filter coefficient as particle deposit causes an increase in surface area available for future particle collection; a decrease in particle filtration as pore spaces are filled and virgin surface

area available for particle collection decreases; and decrease of particle collection as the fluid velocity within the pores increases due to constriction caused by deposition.

Alternatively, the adhesion efficiency (α) can be modified as the deposition progresses to reflect the change in the filter coefficient λ. The level of α is controlled by cell-solid interactions and by the amount of previously attached particle (bacteria). An attached bacterium can reduce the deposition by blocking a part of the collector surface. An expression for the influence of cell-solid interactions and cell-cell interactions (blocking) on α was given by Rijnaarts et al. (1996)

$$\alpha = \alpha_0(1 - B\theta) \tag{2.11}$$

where

α_0= clean bed collision efficiency,

B = blocking factor

θ = fraction of surface covered, i.e. the number of the cells.

Initially, $\theta = 0$ and α is solely determined by cell-solid interactions; $\alpha_0 = 1$ when these interactions do not inhibit the adhesion step. B accounts for the screening of the solid surface by attached cells, i.e. it is the ratio of the blocked area to the geometric area of the cell. It is related to the maximum surface coverage θ_{max} for single layer adhesion: $\theta_{max}= 1/B$. The B factor may vary between 1.5 to more than 20 and depends on geometric or hydrodynamic parameters a_b and N_{pe} and particle-particle interactions (Dabros, 1993 and Admczyk et al, 1992).

2.3.2 Large Scale Bacterial Transport Models

Attempts have been made (Corapcioglu and Haridas, 1985; Harvey and Garabedian, 1991; Hornberger et al., 1992) to model microbial transport through subsurface aquifers with varying degree of success. All of these models use advection-dispersion-reaction

equation where reaction term was appropriately modified to account for deposition, detachment, growth and death of bacteria. Deposition and detachment were mostly incorporated in a similar form as the mass balance equations described above (Equations 2.8 and 2.9). Growth and death were modeled using Monod kinetics and first order endogenous respiration, respectively.

2.3.3 Bacterial Transport Experiments

In order to investigate the various mechanisms affecting bacterial attachment, a number of laboratory studies, involving passage of bacterial solutions through columns packed with sand, Teflon grains, glass beads etc., were conducted (Rijnaarts et al., 1996 a and b; Fontes et al., 1991; Scholl and Harvey, 1992; Martin et al., 1992; Smith et al., 1985; Gannon et al., 1991). The parameters studied were the size distribution and surface properties of collectors (Sand, Teflon and Glass beads etc.), size and surface properties of bacteria and, the pH and ionic strength of water.

An increase in grain size resulted in a decrease of total surface area and hence the bacterial adhesion (Fontes et al., 1991). Bacteria with negatively charged surfaces were adsorbed more when the adsorbent was made positively charged (Scholl and Harvey, 1992). Increase in the ionic strength of the groundwater increased the attachment by double layer compression (Martin et al., 1992; Fontes et al., 1991). Studies at different pHs showed that bacteria retention was higher at lower pH and decreased with increasing pH (Goldschmid et al., 1972; Scholl and Harvey, 1992). Gannon et al., 1991 studied the effect of the size and surface properties on their transport. Bacterial attachment was statistically related to cell size, with bacteria shorter than 1 μm usually showing higher percentages of cells being transported through the soil. Other important parameters governing the attachment and transport of bacteria were reported to be surface charge and hydrophobicity (Sharma et al., 1985; Rijnaarts et al., 1996).

Chapter 3

Scope of Work

From the literature survey, it is clear that the transport of bacteria through the porous media is controlled by many different physical parameters such as, advection, dispersion, diffusion, size and heterogeneity of pore spaces etc. and body forces such as, gravitation, buoyancy, hydrodynamic drag, Van der Waals interaction, electrostatic interaction, hydrophobic forces etc. It is very difficult to perform experiments with porous media to study the effect of each of the individual parameters on the bacteria transport process. In addition, it is difficult to replicate these experiments exactly as the pore space geometry, tortuosity and flow condition will vary each time the porous media is packed anew. It is also difficult to alter one of these interactions independently in the experiments to study the effect, e.g. altering surface characteristics for electrostatic interaction will also alter the hydrophobic interaction. If a computer model can simulate the characteristics and physics of bacterial transport through porous media, some of these experiments can be replaced by simulation or the model can be used to design experiments in a logical way. With this objective in mind, the goal of the present work was set as follows:

- Construct a porous media network model for transport of colloid under saturated flow condition.
- A numerical simulation study for bacteria transport in the porous media using the network model.
- Numerical simulations to study the effect of various properties of porous media and different hydraulic conditions on the breakthrough of bacterial transport through a column.

Chapter 4

Model Building

4.1 Network Model

4.1.1 Spatial Network

The square network was chosen for the present study because it is relatively easier to implement flow and transport models on a square network. However same framework can be used to model other type of networks. The nodes of the network and the tubes connecting them were given the position numbers separately starting from the lower left-hand corner (Figure 4.1). The flow in the network is from bottom to top. Size of the network was $m \times n$ where, m is the number of nodes in the horizontal direction (cross section of the column) and n is the number of nodes in the vertical direction (length of the column).

4.1.2 Pore Throat (Tubes) Radius Distribution

Radius of each pore throat in the network was determined using truncated Weibull distribution function restricted in ($b_{t\,\min}$, $b_{t\,\max}$). Cumulative density function of truncated Weibull distribution function is given as follows (Ioannidis and Chtazis, 1993):

$$F_t(b_t) = \begin{cases} 0, & b_t < b_{t\,min} \\ \dfrac{\exp\left[-\left(\dfrac{b_t - b_{t\min}}{\alpha_t}\right)^{\beta_t}\right] - \exp\left[-\left(\dfrac{b_{t\max} - b_{t\min}}{\alpha_t}\right)^{\beta_t}\right]}{1-\exp\left[-\left(\dfrac{b_{t\max} - b_{t\min}}{\alpha_t}\right)^{\beta_t}\right]}, & b_{t\min} \le b_t \le b_t \\ 1, & b_t > b_{t\,max} \end{cases}$$

where,

$b_{t\,\min}$ = minimum pore throat radius,

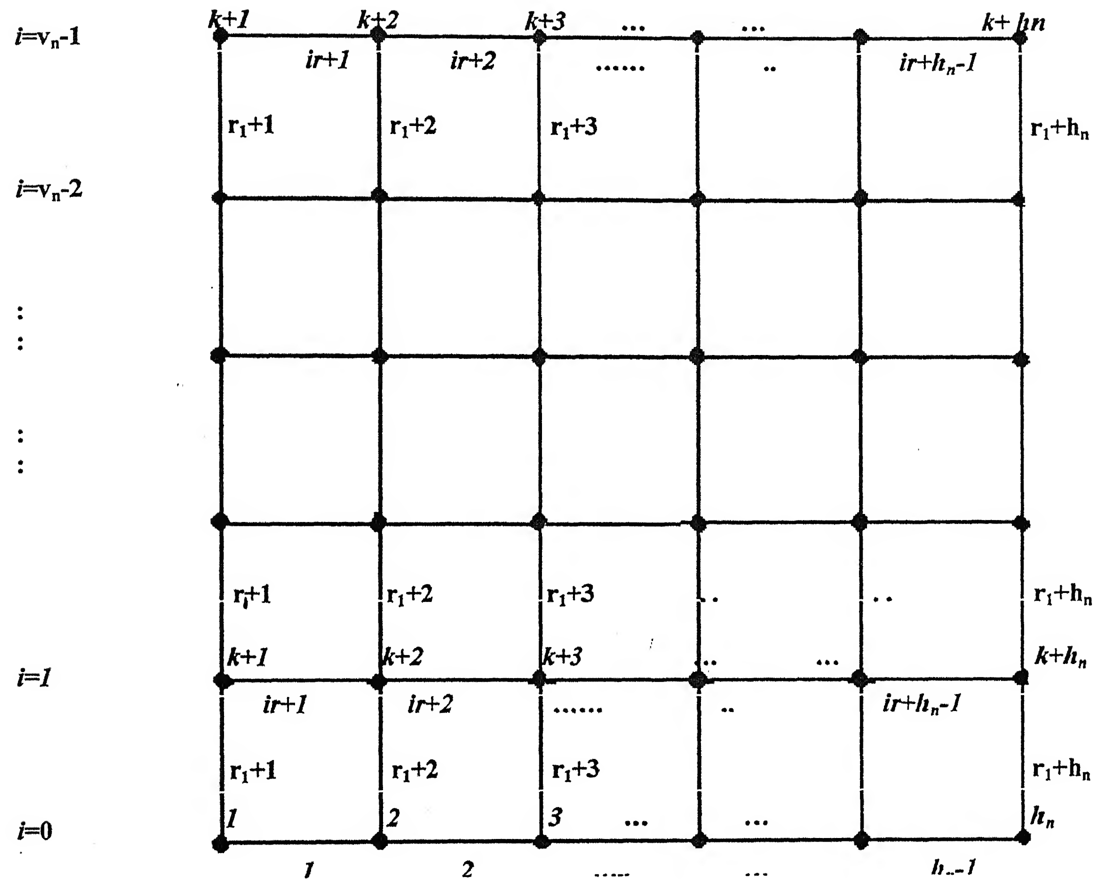

Figure 4.1 Number sequence scheme for the nodes and the tubes of the square network.
h_n = number of horizontal nodes
v_n = number of vertical nodes
i = number of horizontal layers in the network column
$k = ih_n$
$r=2h_n-1$
$r_1=ir+(h_n-1)$
Total number of nodes $= h_n v_n$
Total number of tubes $= h_n (v_n-1)+v_n (h_n-1)$

$b_{t\,max}$ = maximum pore throat radius,

b_t = random number obtained from the distribution and

α_t and β_t = parameters of Weibull distribution.

A random number generator (Hull and Dobell, 1962) was used to obtain the random numbers from a uniform distribution U(0,1). The random numbers obtained from the uniform distribution were transformed to the truncated Weibull distribution using the following transformation equation:

$$b_t = b_{t\,\min} + \alpha_t\left[-\ln\left(R_U(1-A)+A\right)\right]^{1/\beta_t} \tag{4.2}$$

where,

R_U = random number obtained from the uniform distribution in (0,1) and

$$A = \exp\left[-\left(\frac{b_{t\,\max} - b_{t\,\min}}{\alpha_t}\right)^{\beta_t}\right]$$

Thus, a set of independent random numbers having a distribution given in Equation 4.1 was obtained. A total of N_t (number of tubes in the network) random numbers were generated and was assigned sequentially to the tube numbers in the network (Figure 4.1). This way, the radii of the tubes were spatially randomly distributed in the network. The ranges of different parameters of distribution used in this study are shown in Table 4.1.

Table 4.1 Input to get Radius of the Tubes

Parameters	Values	References
α_t	1.0	Ioannidis, 1993
β_t	2.0	Ioannidis, 1993
$b_{t\,min}$	25 μm	Wan and Wilson, 1994
$b_{t\,max}$	50 μm	Wan and Wilson, 1994

4.1.3 Pore Throat (Tubes) Length

Lengths of the tubes were constant in the regular network. Depending on the soil type, either the length of the pore throat or the porosity of the network was supplied. If the porosity of the network was supplied as input then the pore throat length was calculated and if the length was supplied then the porosity of the network was calculated. The calculation was based on the aerial porosity as a two-dimensional network was assumed to be similar to an interface, a limiting case of a three dimensional network when one of the dimension approaches zero (Hassanizadeh and Gray, 1979). The mathematical relation between length of the pore throat (tubes) and the porosity of the network was as follows:

$$l = \frac{2\sum_{i=1}^{N_t} R_i}{\varepsilon (h_n - 1)(v_n - 1)} \tag{4.3}$$

where,

l = length of one tube,

R_i = radius of ith tube,

ε = porosity of the network,

h_n = number of horizontal nodes,

v_n = number of vertical nodes,

N_t = total number of tubes in the network.

4.2 Flow Through the Network

4.2.1 Pressure Head at Nodes

The head loss was calculated at each tube of the square network model using Darcy-Weisbach equation.

$$h_{ki} = \frac{flv_{ki}^2}{4gR_{ki}} \tag{4.4}$$

where,

h_{ki} = head loss in the tube connecting nodes k and i,

v_{ki} = velocity in the tube connecting nodes k and i,

f = friction factor,

R_{ki} = radius of the tube connecting nodes k and i.

The above equation for a single tube connected between the nodes k and i can be written as:

$$h_{ki} = H_k - H_i = K_{ki} sign(Q_{ki})|Q_{ki}|^{n_{ki}} \tag{4.5}$$

where,

K_{ki} = head loss coefficient for the tube connecting nodes k and i, $= \dfrac{fl}{4\pi^2 g R_{ki}^5}$ for $n_{ki} = 2$

H_i = head at the ith node,

Q_{ki} = discharge in the tube connecting the nodes k and i,

n_{ki} = exponent in the head loss equation for the tube connecting nodes k and i,

Since the head loss is positive in the direction of flow, sign of the head loss is same as sign of the flow. So the Equation 4.5 can be inverted as follows:

$$Q_{ki} = sign(H_k - H_i)\left(\frac{|H_k - H_i|}{K_{ki}}\right)^{1/n_{ki}} \tag{4.6}$$

The continuity equations for the node i in the network can be written as follows:

$$\sum_{k=1}^{m_i} Q_{ki} = U_i \quad \text{for } i = 1, 2, 3 \cdots\cdots N_t \tag{4.7}$$

where,

U_i = consumptive use at node i,

m_i = number of connections to node i.

The energy and continuity equations can now be combined as follows taking $U_i = 0$ for each node i:

$$\sum_{k=1}^{m_i} sign(H_k - H_i)\left(\frac{|H_k - H_i|}{K_{ki}}\right)^{1/n_{ki}} = 0 \quad \text{for } i = 1, 2, 3\cdots\cdots\cdots N_t \tag{4.8}$$

There is one such equation for each node and the variables are heads (H_i's) at each node. So, this gives a system of non-linear simultaneous equation of size $h_n v_n - 2h_n$, where $h_n v_n$ is the total number of nodes in the network. This system of non linear equations were solved using Newton-Raphson method. Only the heads at the inlet boundary and the outlet boundary were supplied. This is equivalent to supplying the difference in head between inlet and outlet of a column or the pressure drop in a column.

4.2.2 Discharge in the Tubes

The net discharge Q_{ki} in each tube connecting nodes k and node i was calculated from the Equation 4.6.

4.2.3 Velocity of Fluid in Tubes

The net velocity of fluid in each tube was calculated from the net discharge in the tube and the cross-sectional area of the tube.

$$v_{ki} = \frac{Q_{ki}}{\pi R_{ki}^2}$$

where,

v_{ki} = Flow in the tubes connecting the nodes k and i.

4.3 Bacteria Transport Model

4.3.1 Inflow Concentration

After determining the velocity of the flow in all the tubes of the network the influent concentration $C_0 = 0.005$ kg/m^3 was added to the fluid going into the network. In all the tubes placed at the bottom layer of the network having the position number h_n to $2h_n$-1 were given an initial concentration $C_0 = 0.005$ kg/m^3 and the rest of the tubes were having $C_0 = 0$ at time $t = 0$. It may be noted that in this study, SI system was used for unit of all the parameters. If the influent bacteria concentration is defined alternatively as the number of cells per 100 mL, the values and units of all other parameters need to be changed accordingly.

4.3.2 Effluent Concentration and Bacterial Deposition

The tubes in the network are very small in length. For small time step (Δt), λ may be considered independent of x and t in each tube during every time step. This enables the Iwasaki equation (Equations 2.4 and 2.5) to be applied to individual tubes for the calculation of effluent concentration. In the Equation 2.5, the λ_0 was substituted by λ and it was modified after every time step using Equation 2.5. The influent concentrations (C_{0t}) were the concentrations at the influent nodes of the tubes and changed at every time step depending on the concentrations at various nodes.

For the calculation of σ, detachment or scouring can be neglected ($s = 0$) as bacterial deposition is often considered to be irreversible (Rijnaarts et al. 1995, Sjollema et al. 1990). The deposition (σ) can be obtained by combining the Iwasaki Equation 2.4, and Equation 2.8 and by substituting λ for λ_0 to take into account the time dependence. It is possible to obtain a closed form solution of Equation 2.8 for a small time step in a small tube (constant λ), as follows (McDowell-Boyer, 1986):

$$\sigma = UC_{0t}\lambda e^{-\lambda x} t \qquad (4.10)$$

where,

C_{0t} = influent concentration of the tube, updated every time step.

Due to deposition, the porosity of the network changes. Hence the velocity was also modified at each step using the relation:

$$v = v_0(1-\sigma) \qquad (4.11)$$

The maximum deposition was taken as 10% in the present study.

The effluent concentration was calculated at the end of each time step (Δt) from the individual tube using the Equation 2.5 with the updated value of λ and C_0 is taken as the inflow concentration in the tube at that time. The final effluent concentration from the column of the network was net concentration of out flow from the vertical tubes at the upper end.

4.3.3 Filter Coefficient

The initial filter coefficient (λ_0) was calculated for each tube using the Equation 2.7. The values of the filter coefficients (λ) were modified using Equation 2.10 after every time step (Δt) for each tube.

4.4 Numerical Scheme of Solution for Breakthrough Curve of Bacterial Transport

Flow chart of the whole network model is shown in Figure 4.2. A detailed outline of the time stepping scheme involved in the calculation of effluent concentration (C) and deposition (σ) is given below:

Step 1: The minimum time taken by the fluid coming from the bottom layer, to reach each of the nodes of the network was calculated. Hence each node was associated with the minimum time T_{min}.

Step 2: To determine the concentration profile the time step Δt was chosen.

Step 3: Concentration of the particle was calculated at each node after the time step Δt. If T_{min} at any node is greater than Δt, then concentration at that node was taken as zero.

Step 4: After each time step Δt, the total deposition in the tube was calculated, the velocity of the fluid in the tubes was modified due to the bacterial deposition and the new filter coefficient (λ) was calculated.

Step 5: At each node the concentration was determined and effluent concentration was calculated.

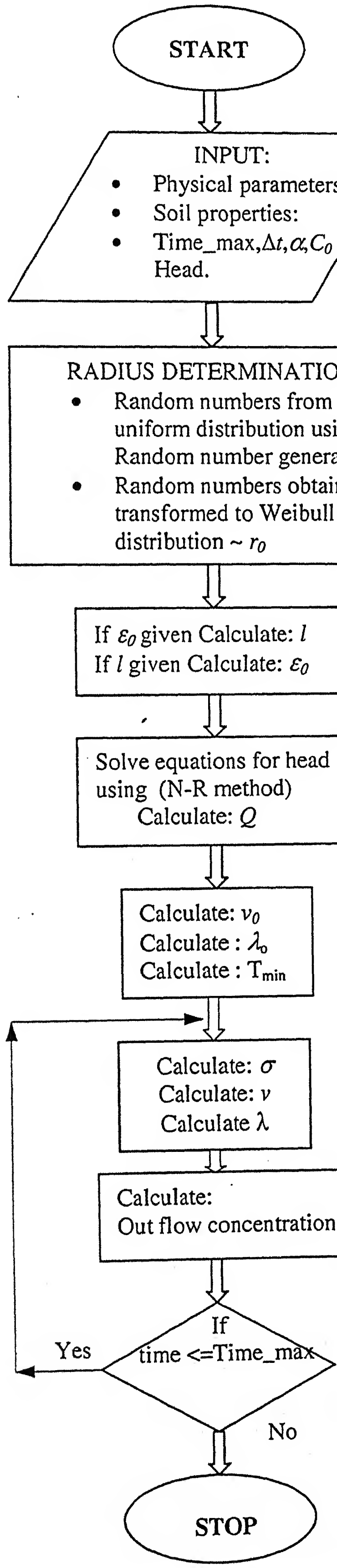

Figure 4.2 Flow chart representing the steps involved in bacterial transport model

Chapter 5

Results and Discussion

5.1 Generation of Porous Media Network

5.1.1 Effect of α_t on the Radius Distribution

The effect of α_t on the radius distribution is shown in the Figures 5.1a-b. For a constant value of $\beta_t = 2.0$, the radii distributions were compared for $\alpha_t = 0.1$ and $\alpha_t = 1$. The shape of the distribution curve was observed to remain same in both the cases but it was shifted towards higher radius values.

5.1.2 Effect of β_t on the Radius Distribution

The effect of β_t on the radius distribution is shown in the Figures 5.2a-b. For a constant value of α_t =1.0, the radii distributions were compared for β_t = 1.0 and β_t = 4.0. The values of β_t are related to the shape of the distribution curve. For the higher values of β_t (= 4.0) the distribution was more symmetric and narrower compared to that with the lower value of β_t (= 1.0).

5.1.3 Effect of $b_{t\,max}$ and $b_{t\,min}$ on the Radius Distribution

The parameters $b_{t\,\max}$ and $b_{t\,\min}$ determine the mean pore size as well as the range of the distribution and are directly related to the soil type. For example, sandy soil is likely to have bigger pore sizes compared to those of clay soil. Three different ranges of pore size distribution with same α_t and β_t values are shown in Figures 5.1b and 5.3a-b. These distributions were generated by changing the values of $b_{t\,\max}$ and $b_{t\,\min}$.

5.1.4 Validation of Porous Media Network through Pressure Saturation Curve

Generation of pressure saturation curve does not require solving the hydraulic model or the transport model. It can be directly obtained from the network properties (Fatt, 1956). For

the present study, the value of α_t and β_t were taken as 1.0 and 2.0, respectively. The relation between capillary pressure and wetting phase saturation is shown in Figure 5.4. The network data gives the stepped curve because the radius distribution is not continuous. In real porous media with continuous pore throat radius distribution, the capillary pressure saturation curve is always smooth. In Figure 5.4, the dashed line shows the result of smoothing the network data. The relation obtained from the network model resembles a typical capillary pressure curve with the exception that the curve derived from the network is asymptotic to zero wetting phase saturation, whereas curve from real porous media is asymptotic to 20 to 30 percent wetting phase saturation (residual saturation). This difference is due to the dead end pores in the real porous media that can trap fluid during drainage. However, the curve matches with other reported results from network model (Fatt, 1956).

5.2 Hydraulic Model

The hydraulic model was tested with small network sizes of 3×3 and 3×4. The values obtained from the program were compared to the manually calculated values. It was tested for both constant tube radii and radii distribution obtained from Weibull distribution. The simulated heads at the nodes and the corresponding discharges in the pipes matched the computed values exactly. Figure 5.5a and b shows a typical result.

5.3 Bacterial Transport Model

Following the confirmation of the porous media network model and hydraulic model, the bacterial transport model was incorporated in the network. The following sections describe the verification of the bacterial transport model for consistency.

Table 5.1 Input supplied

Parameters	Notation	Values	References
Particle diameter	d_p	1×10^{-6} m	Basu, 2001
Grain diameter	d_m	0.54×10^{-3} m	Basu, 2001
Relative particle density	ρ_p	1.05	Basu, 2001
Fluid density	ρ_f	1.0×10^{3} kg/m^3	Basu, 2001
Friction factor	f	0.05	Subramanya 2000
Diffusivity	D_p	4.3×10^{-13} m^2/sec	McDowell-Boyer, 1986
Initial Porosity	ε_0	0.4	Basu, 2001
Initial bacteria concentration	C_0	0.005 kg/m^3	Basu, 2001
Fluid dynamic viscosity	μ	0.00098 N-s/m^2	McDowell-Boyer, 1986
Empirical parameters	x', y', z', β	1.0	

5.3.1 Effect of Time Step on the Breakthrough Curve

The choice of time step plays a critical role in the transport model. If the time step chosen is larger than the smallest flow through time in one of the tube of the network, deposition of particles will be time-lumped in more than one tube. The effect of time step on the breakthrough curve obtained from the network is shown in Figure 5.6. For this simulation, a network size of 10x10 and conservative tracer ($\alpha = 0$ in Equation 2.7)

was used. The breakthrough curves became invariant of the time step beyond 2.5×10^{-6} sec. Based on this result, the time step was taken as 2.5×10^{-5} sec for all the simulations.

5.3.2 *Effect of Cross Section of the Column*

The breakthrough curve is expected to be invariant of the column cross sectional area. This was checked by keeping the number of vertical nodes fixed at 10 and expanding the network horizontally by increasing the number of nodes from 10 to 50. The simulations were once again conducted for a conservative tracer with zero retention. Figure 5.7a shows the results of these simulations. As expected, the breakthrough curves remain invariant of the column cross section. The network model imparts dispersion in the breakthrough curve (Figure 5.7a) evident from the gradual variation of the effluent concentration before it reaches the influent concentration. This is typically observed in the experiments (Fontes et al., 1991; Harvey and Garabedian 1991). Simple application of the Iwasaki Equation (2.4) to a single tubular column reactor will give no dispersion. This indicates that a network model is capable of producing results that is characteristically similar to the experimental results.

5.3.3 *Effect of Length of the Column*

Increasing the length of the column is likely to delay the initial breakthrough as well as impart more dispersion (Fontes et al., 1991; Harvey and Garabedian 1991). In the simulations, the number of horizontal nodes was kept fixed as 10 and the network was expanded vertically by increasing the number of nodes from 10 to 50. Once again, the simulations were conducted on a conservative tracer. The effects of increasing the number of nodes in the vertical direction on the breakthrough curve are shown in the Figure 5.7b. As expected, the time for initial breakthrough as well as the dispersion increased with increasing length of the column.

5.4 Comparison of Simulated Results with Experimental Results

A set of experiments was reported (Rijnaarts et al. 1996) for bacterial transport through same media but different lengths of column. The model simulation was conducted to see how a 2-d network model simulates the results obtained from 3-d column experiments. The pore size distribution as well as the adhesion efficiency (α) was unknown. The pore size distribution was obtained by taking α_1 =1.0 and β_1 = 2.0. The adhesion efficiency was assumed as unity. Simulation results (Figure 5.8a) were compared to the experimental results (Figure 5.8b). The time scale of breakthrough was much smaller in the 2-d network than the experiments as the pore volume of the network is much less and an added dimension in the columns gives the pores more connectivity and tortuosity. However, similarity of the effect of column length on the breakthrough levels of C/C_0 is evident. The point at which C/C_0 reached a plateau decreased with increasing column length similarly in simulations and experiments.

5.5 Effect of Different Physical Parameters

5.5.1 Effect of Porosity

In order to study the effect of porosity, a network of dimension 10×100 was taken and the porosity was changed keeping all other parameters of the model constant. The comparison of the breakthrough curves for three different porosities 0.3, 0.4 and 0.5, is shown in Figure 5.9. It shows that for the same soil type and bacteria, a well-consolidated bed of soil will transport higher amount of bacteria due to lower pore space available for deposition.

5.5.2 Effect of Flow Rate

For the same column, lower flow rate yields higher hydraulic retention time. This is equivalent to increasing the length of the column for the same flow rate. So, the effect

of decreasing the flow rate is same as increasing the length of the column and is demonstrated in Figure 5.10 for a 10 × 100 network.

5.5.3 Effect of $\sigma_{v\,max}$

Another parameter that is very hard to determine experimentally is the maximum specific deposit ($\sigma_{v\,max}$) beyond which the no more bacterial deposition is possible. As a result, it is impossible to set a value of $\sigma_{v\,max}$ for simulation. This set of simulation was conducted to see the effect of the value of maximum specific deposit on the final breakthrough curve. It is easily seen that the variation, although present, is not very significant (Figure 5.11). A decrease of one order of magnitude to the value of $\sigma_{v\,max}$ resulted in less than 10% difference in the breakthrough curve. Although, it is expected that, at the lower values of $\sigma_{v\,max}$, the result will be more sensitive since, λ approach infinity as $\sigma_{v\,max}$ approach zero Equation 2.10.

5.5.4 Effect of Adhesion Efficiency (α) and Mass Transfer Efficiency (η)

At present, no model or description exists for the adhesion efficiency (α). It is often chosen arbitrarily. Rijnaarts et al. (1996) proposed various ways to compute the adhesion efficiency from the breakthrough curves of column experiments but the results varied depending on the method used. As a result, it is impossible to set this parameter for any simulation. A sensitivity study was conducted to observe the effect of α on the breakthrough curve (Figure 5.12). For the full range of α (0 to 1), the breakthrough curves vary significantly indicating the adhesion efficiency to be an important parameter. Since, the mass transfer efficiency and the adhesion efficiency are multiplied to each other in the expression of the filter coefficient (Equation 2.7), the breakthrough curves are equally sensitive to the mass transfer efficiency.

5.6 Application Perspective

Application of the 2-dimensional network model is in designing column experiments for the colloid transport through a packed bed or porous media. The model is capable of predicting trends as well as variations of the breakthrough curves under different parameters and conditions. This will help in deciding the key control variables and parameters for the design of colloid transport experiments in porous media. Thus, it will reduce the number of experiments to be conducted. Expanding the 2-d model to a 3-d network is possible but the computational requirement may outweigh the advantage of conducting less number of experiments. The change from a 2-d to a 3-d network is unlikely to provide any added insight into the mechanism of problem. Lastly, calibration of the network model pȧrameters with experimental data may enable the model to be used as a predictive tool.

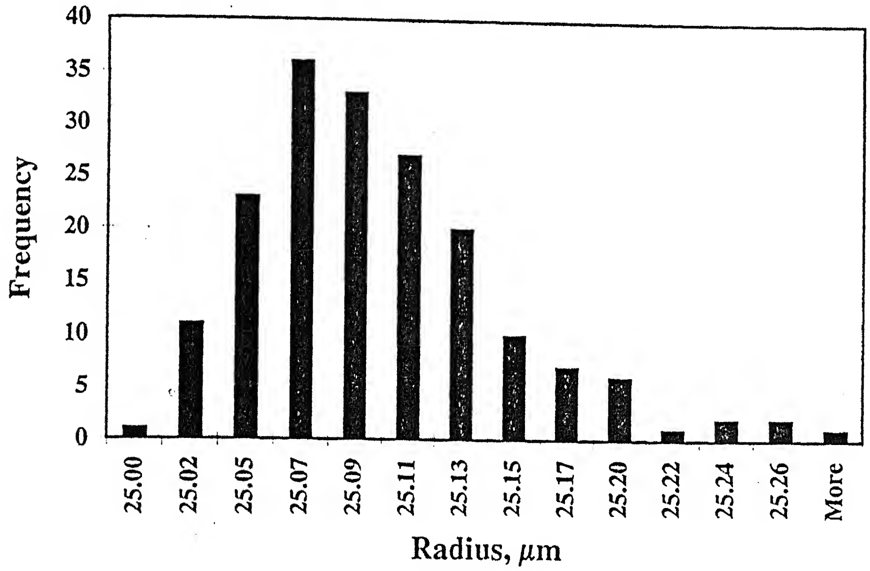

Figure 5.1a Effect of distribution parameters on the radius distribution. b_{tmax}= 50.0 µm, b_{tmin} = 25.0 µm, α_t=0.1, β_t=2.0.

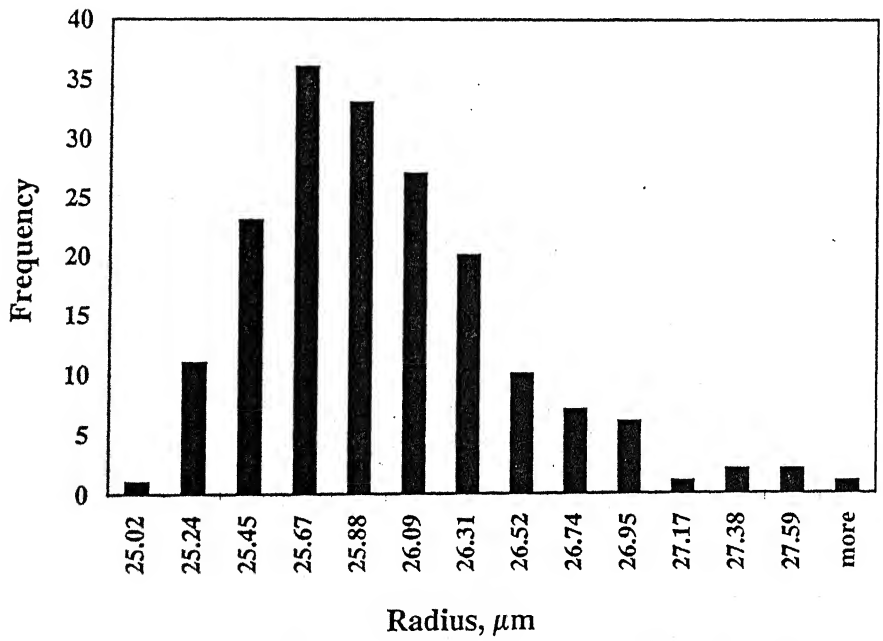

Figure 5.1b Effect of distribution parameters on the radius distribution. b_{tmax}= 50.0 µm, b_{tmin} = 25.0 µm, α_t = 1.0, β_t = 2.0.

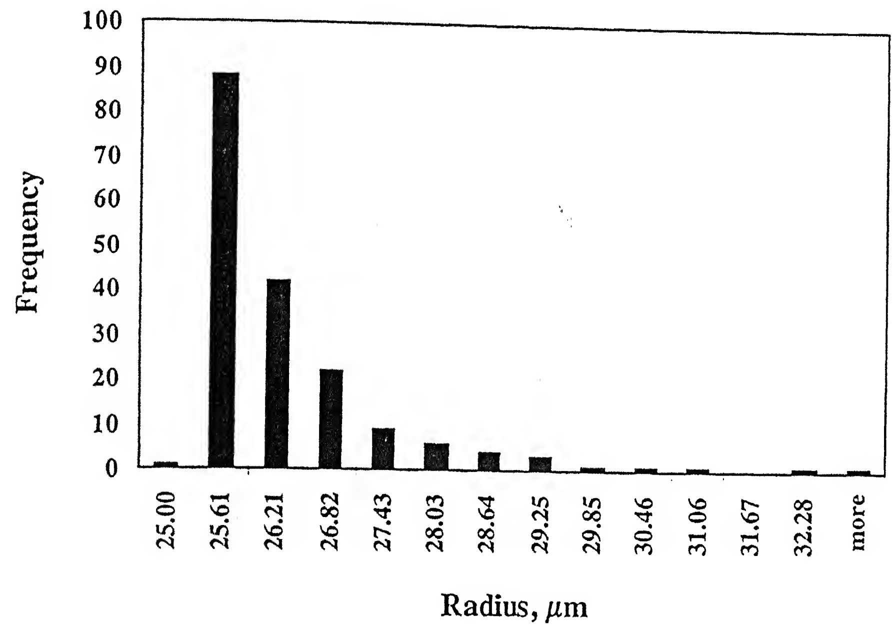

Figure 5.2a Effect of distribution parameters on the radius distribution. $b_{tmin} = 25.0$ µm, $b_{tmax}= 50.0$ µm, α_t=1.0, β_t=1.0.

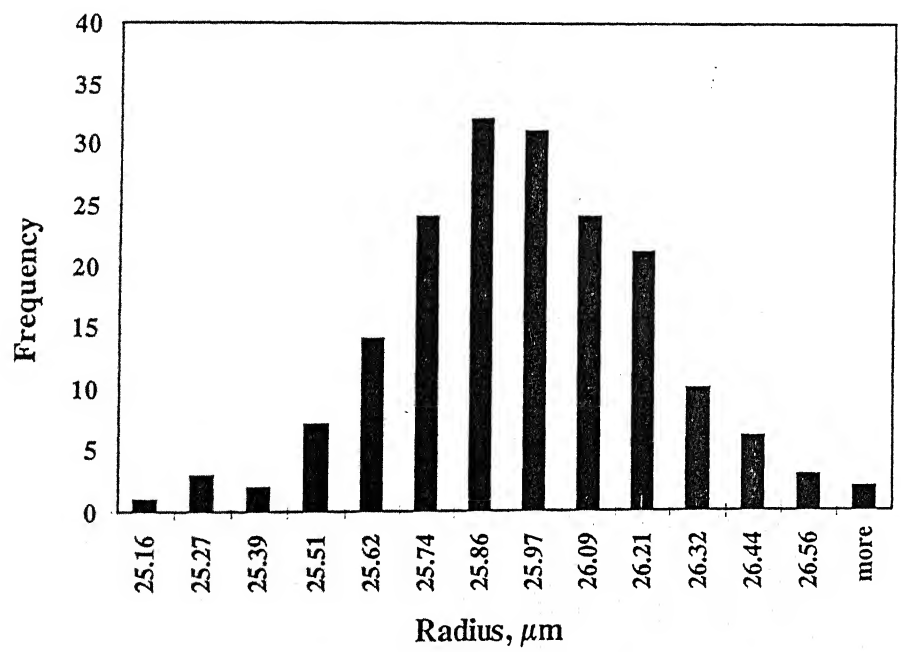

Figure 5.2b Effect of distribution parameters on the radius distribution. $b_{tmin} = 25.0$ µm, $b_{tmax}= 50.0$ µm, α_t=1.0, β_t=4.0

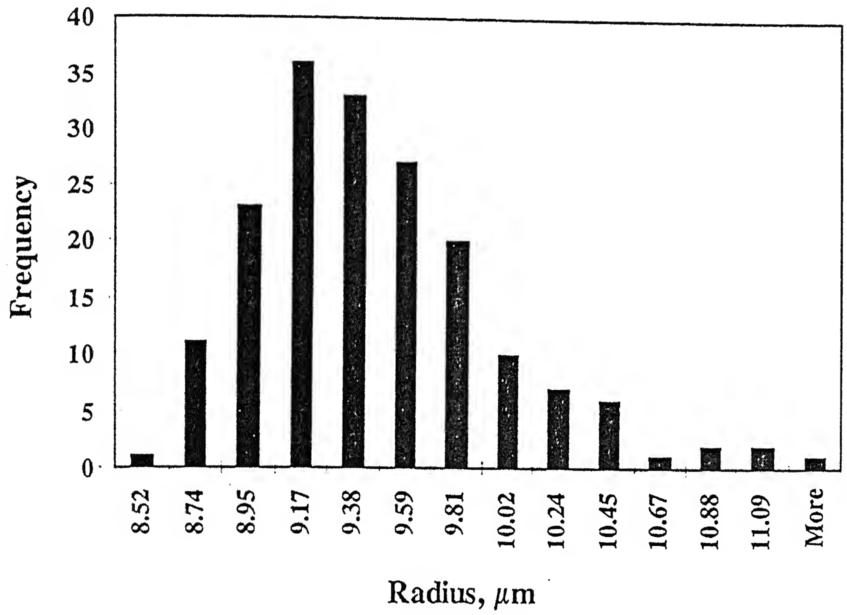

Figure 5.3a Effect of grain size on the radius distribution. b_{tmin}= 8.5 μm, b_{tmax} = 20.0 μm, α_t=1.0, β_t=2.0

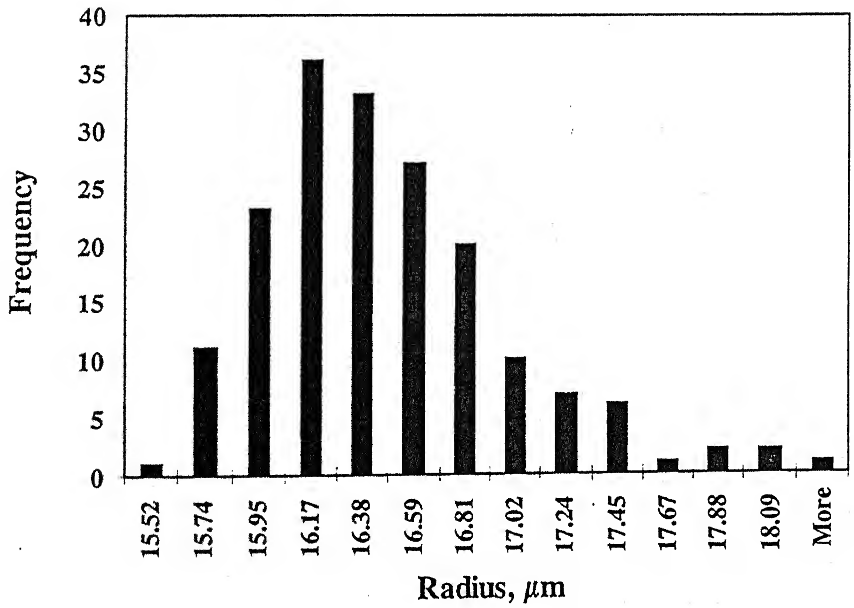

Figure 5.3b Effect of grain size on the radius distribution. b_{tmin}= 15.5 μm, b_{tmax} = 25.5 μm, α_t=1.0, β_t=2.0.

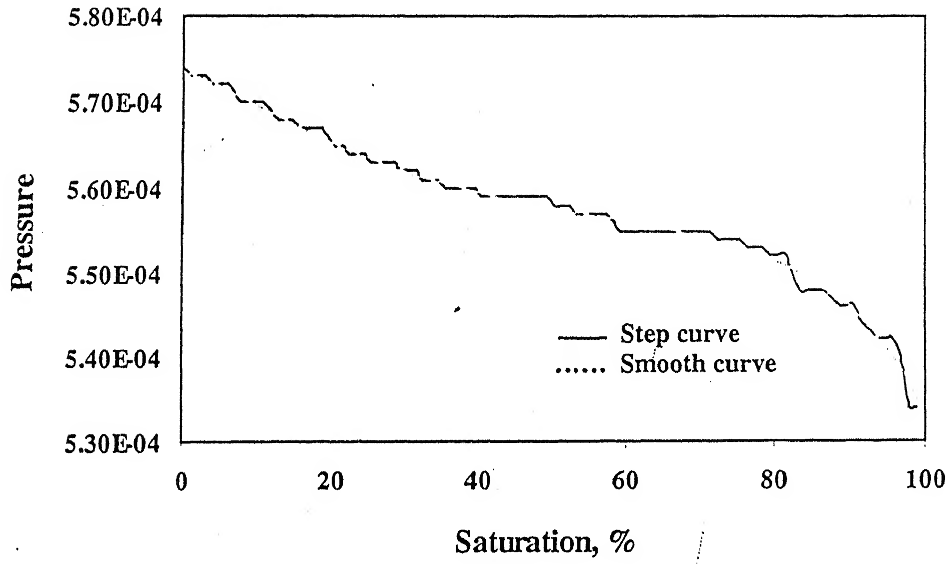

Figure 5.4 Nondimensional capillary pressure characteristics of square network of size 10×10 using radius distribution of Figure 5.1b.

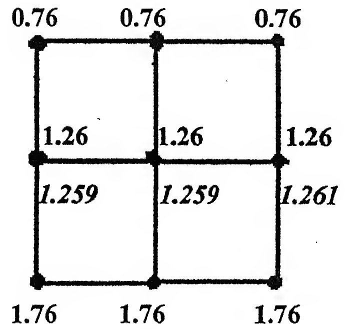

Figure 5.5a Computed values of pressure head for 3x3 Network. Black numbers show the supplied values for the head at the end nodes. Green numbers are computed head at the nodes for the uniform radius network. Blue numbers represent computed head at the nodes for the network having radius distribution obtained from the weibull distribution.

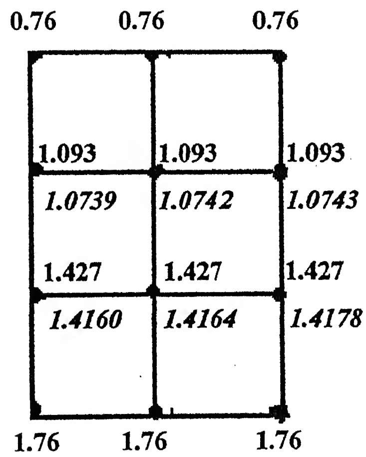

Figure 5.5b Computed values of pressure head for 3x4 Network. Black numbers show the supplied values for the head at the end nodes. Green numbers are computed head at the nodes for the uniform radius network. Blue numbers represent computed head at the nodes for the network having radius distribution obtained from the weibull distribution.

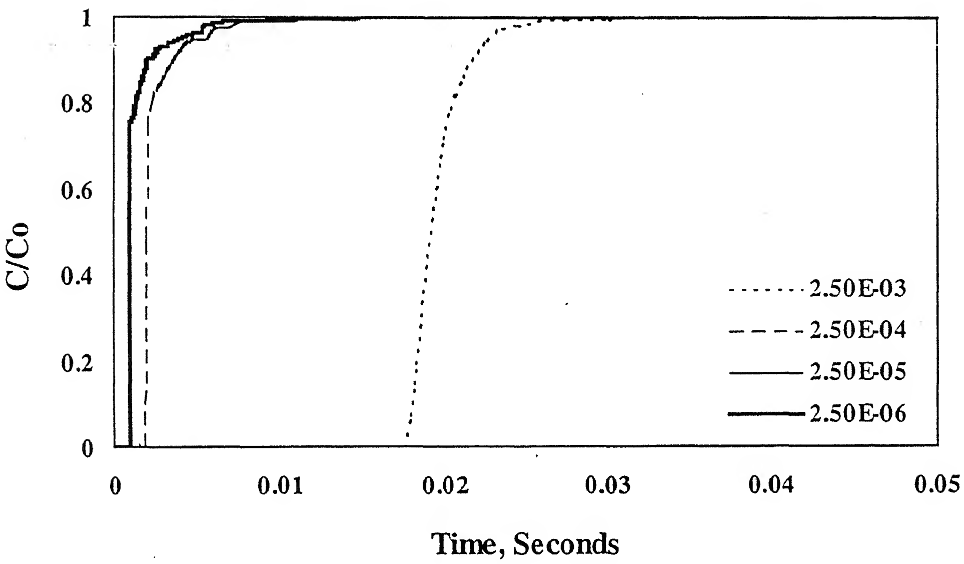

Figure 5.6 Effect of time step on the breakthrough curve for bacterial transport. Network dimension 10×10, Head =1 m, Porosity = 0.4, α =0. Legend shows time step in seconds.

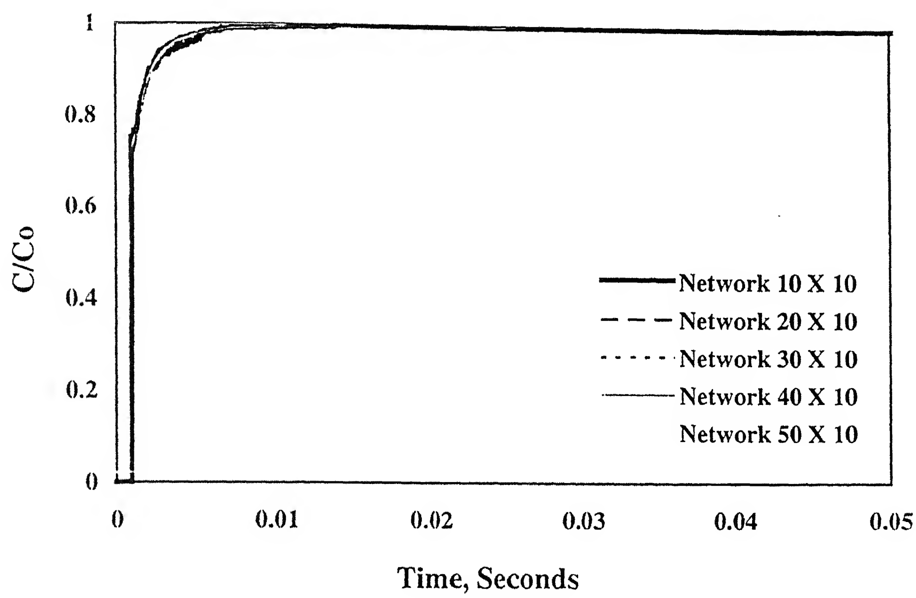

Figure 5.7a Effect of cross section of the network on the breakthrough curve for conservative tracer. Head =1 m, Porosity = 0.4, α = 0, Time step = 2.5E-5.

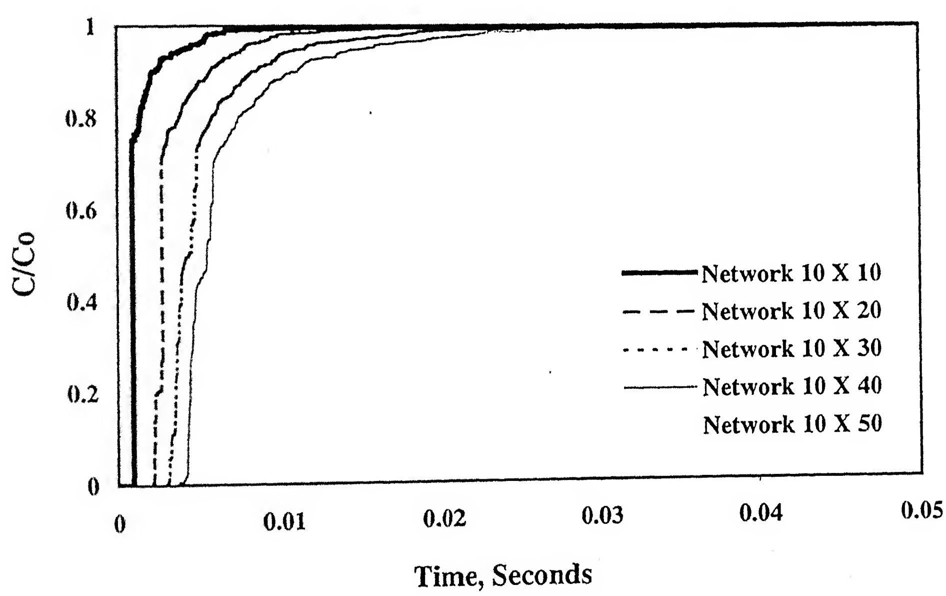

Figure 5.7b Effect of vertical length of the network on the breakthrough curve for conservative tracer. Head =1 m, porosity = 0.4, α = 0, Time step = 2.5E-5.

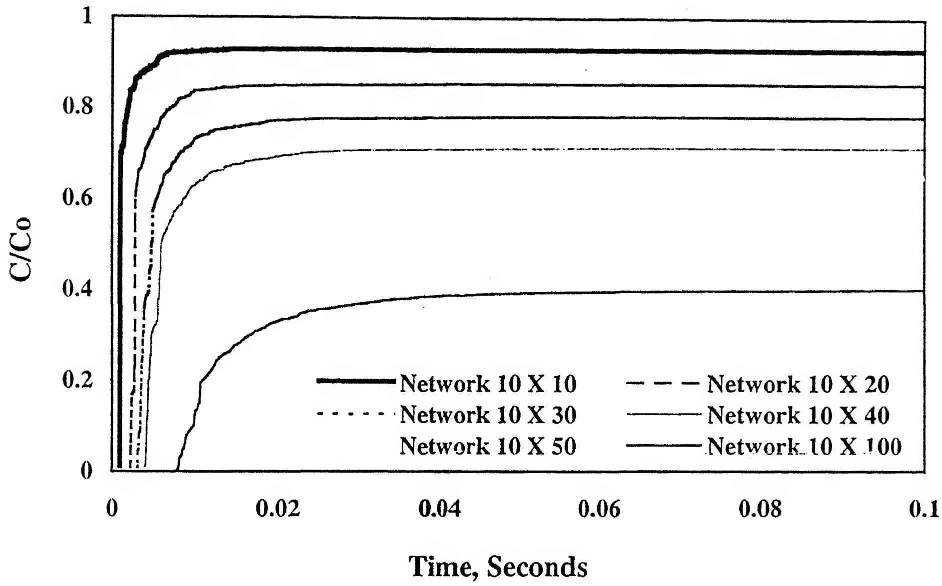

Figure 5.8a Effect of vertical length of the network on the breakthrough curve for bacterial transport. Head =1 m, porosity 0.4, α= 1, Time step 2.5E-5.

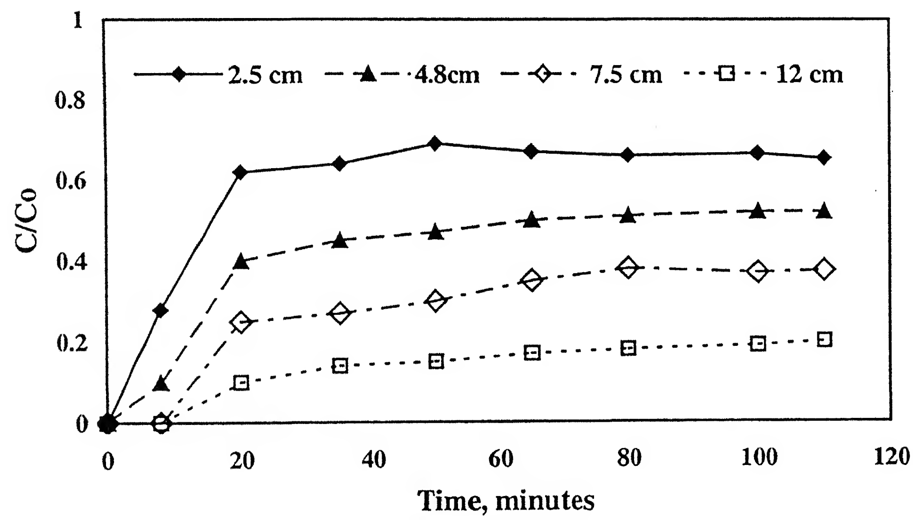

Figure 5.8b Effect of column length on the breakthrough curves for bacterial transport. (Rijnaarts et al., 1996.)

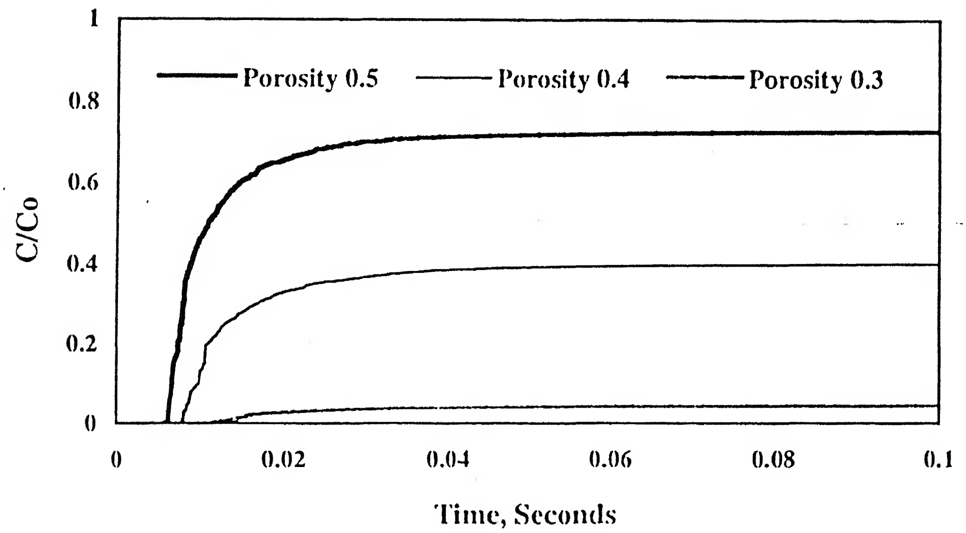

Figure 5.9 Effect of porosity on the breakthrough curve for bacterial transport. Head 1 m, Network dimension 10×100, $\alpha = 1.0$, Time step 2.5E-5.

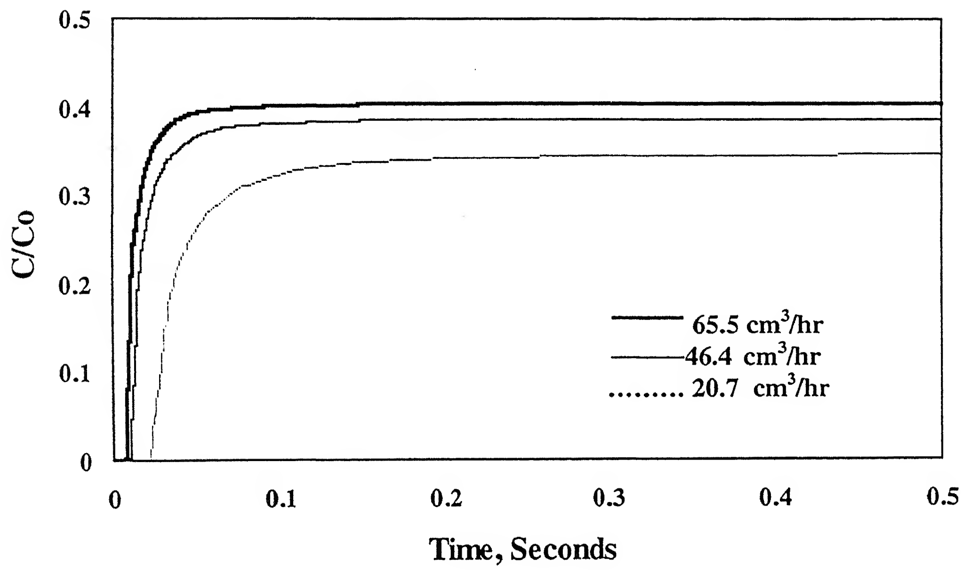

Figure 5.10 Effect of flow rate on the breakthrough curve for bacterial transport. Network dimension 10×100, α= 1.0, Time step 2.5E-5, Porosity = 0.4. Legen shows flow in the network.

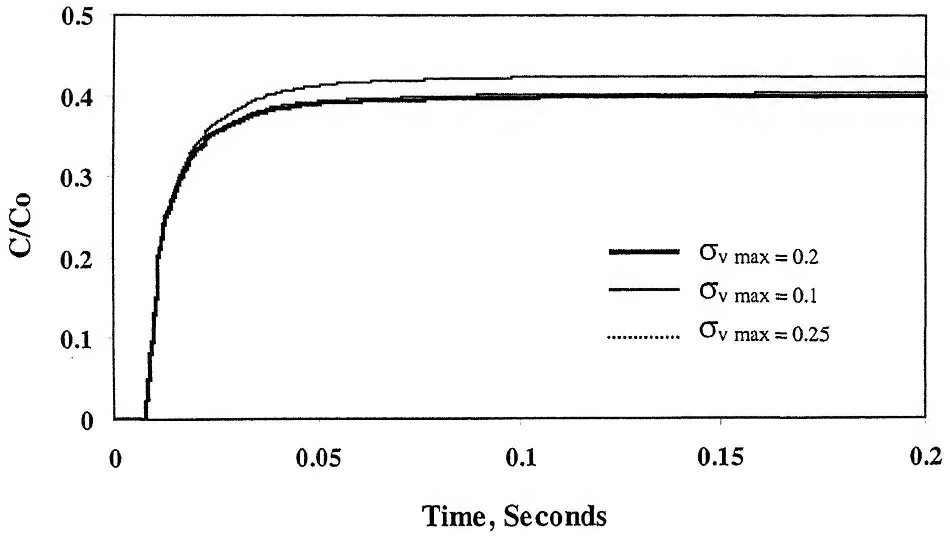

Figure 5.11 Effect of maximum deposition on the breakthrough curve for bacterial transport. Head = 1m, Network dimension 10×100, α = 1.0, Time step 2.5E-5, Porosity = 0.4.

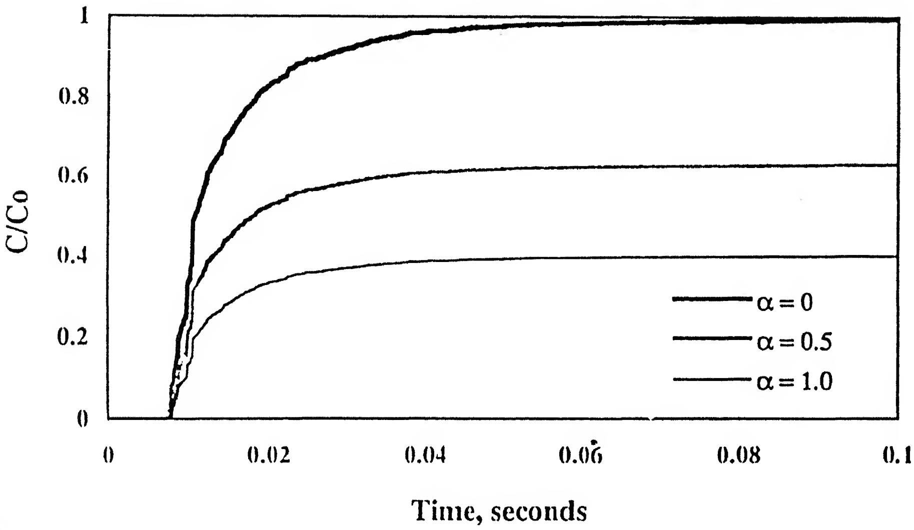

Figure 5.12 Effect of α on the breakthrough curve for bacterial transport. Head =1 m, Network dimension 10×100, Porosity = 0.4, Time step 2.5E-5.

Chapter 6

Summary and Conclusion

The present research was undertaken in two steps. In the first step the two-dimensional network model was developed to represent the porous media. In the second step the bacterial transport study was done. The Weibull distribution function was used to determine the radius of the tubes of the network representing porous media. The network was tested for successful generation of pressure saturation curve. After validating the hydraulic model with the hand-computed values in simple network, the model was used to generate the breakthrough curves for bacterial transport. The following observations can be made from the study:

- The distribution parameters, α_t and β_t play important roles in determining the shape and spread of the pore size distribution. The parameters $b_{t\ min}$ and $b_{t\ max}$ set the range of distribution and their values should be governed by the knowledge of the properties of porous media.
- Choice of time step is an important factor for the consistency of the model results.
- Application of Iwasaki equation over the individual tubes in a network with the consideration that the filter coefficient is constant for a small tube in a small time step, is capable of producing the expected dispersion trends for a conservative tracer.
- The effect of cross section and the vertical length of the column for a conservative tracer produced the expected trends. The breakthrough curve remained invariant with the changing cross section of column. Increasing the column length increased the dispersion.

- For a non-conservative particle (bacteria) transport, the model results simulated the trends of the experimental results.
- In the sensitivity studies, adhesion efficiency (α) was found to be a very important parameter for bacterial transport.

Chapter 7

Scope of Future Work

The Following Areas are recommended for further investigations:

- A Happel's sphere in cell model for the mass transfer efficiency (η) may be incorporated in the network model. This will enable the model to study the effect of different surface forces arising out of various particle and collector surface characteristics.
- A deterministic model for the collection efficiency (α) is needed.

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